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Bridging first-principles calculations together with seismological models

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Almost all the ab inito studies performed so far for various (possible) Earth's inner core materials were conducted by comparing together the computed longitudinal (Vp) and shear (Vs) wave velocities to the first-order velocity term of seismological models. We here demonstrate that further constraints on the Earth's inner core composition can be provided if first-principles data are also compared with the second-order velocity term. The proposed procedure represent a new way to enforce the agreement between existing seismological models and ab initio calculations and provides a more severe way to guarantee the uniqueness of the achieved results.